Molecular theory of weak polyelectrolyte thin films

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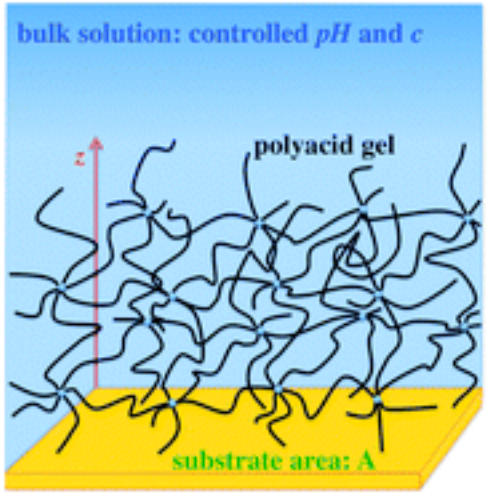
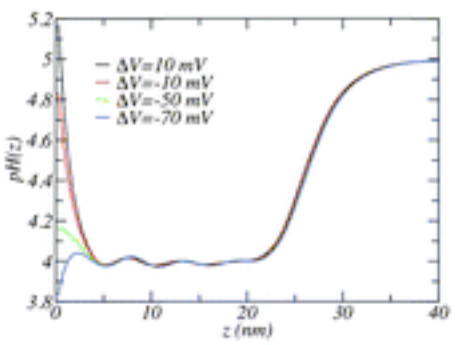
Hydrogels of ionizable polymer chains can swell many times their volume in response to a variety of external stimuli, such as changes in solution pH and ionic strength. Thin hydrogel films are suitable for use in the development of new micro/nano-sized applications requiring fast and stable stimuli-responsive materials.





The local gel pH can be controlled by the applied potential

In this work, we used a Molecular Theory to study the response of a thin film of cross-linked hydrophilic polyacid chains to variations in external stimuli such as pH, salt concentration and applied electric potential. We found that pH in the different regions inside and near the gel can be controlled by changing the bulk pH and salt concentration. In addition, there is a gradient of pH going from the solution inside the film, whose magnitude can be tuned by varying bulk pH and salt concentration. In the region near the surface, both the pH and total charge density can be controlled by applying an electric potential. The thin film behaves as an electric insulating material. We calculated the potential of mean force for the insertion of charged nanoparticles inside the hydrogel film. Depending on the electric charge and size of the nanoparticle, there can be an attractive well or a repulsive barrier of several k_BT for the nanoparticle to enter the gel from the solution. These findings are relevant in the design of a variety of functional devices using hydrogel films.

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